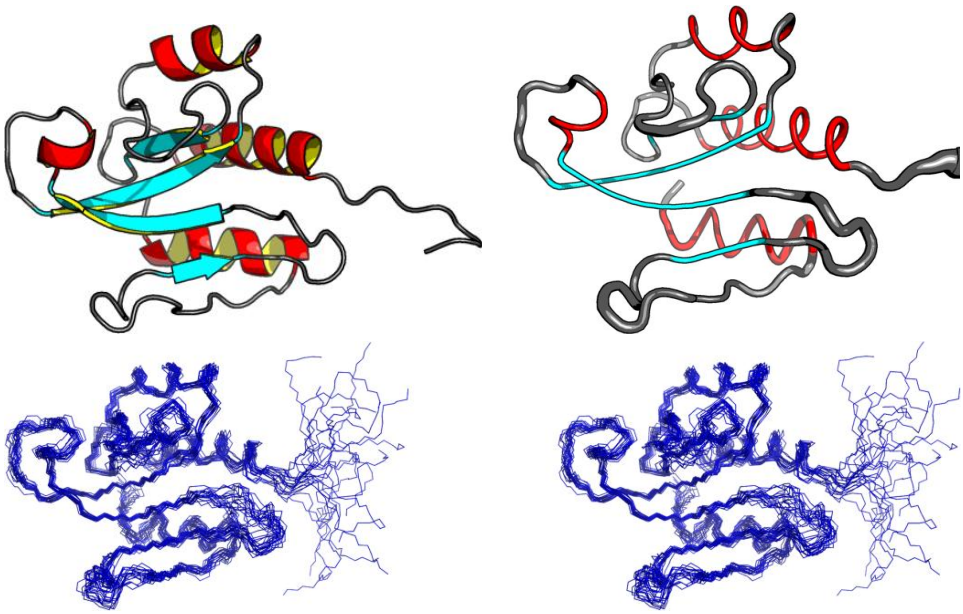
Structure Quality Analysis for NAME

Analyses performed for user defined residues.
The constraints analysis is based on the following files: NOE distance constraints file. Angular constraints file. H-bond constraints file.
Procheck analysis,RMSD calculation and structure superimposition are based on: User defined residues

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	125
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	monomer
Molecular weight:	14802



Secondary Structure Elements:
alpha helices: 3A-14A, 71A-76A, 102A-115A
beta strands: 29A-31A, 41A-47A, 58G-65G, 91P-95P, 80E-82E

Total number of restricting constraints per restrained residue: 17.0
Restricting long range constraints per restrained residue: 4.9
Distance violations per model
Calculated using sum over r^-6

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
7.8	4.7	1

Dihedral angle violations per model

1 - 10 °	> 10 °
2.2	1.6

FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score

0.912 0.839 0.874 0.744

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	2.1 Å	0.8 Å	0.8 Å
All heavy atoms	2.7 Å	1.3 Å	1.3 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
95.6%	4.4%	0.0%	0.0%

Ramachandran Plot Summary for selected residues[3] from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
99.2%	0.7%	0.1%		

Global quality scores

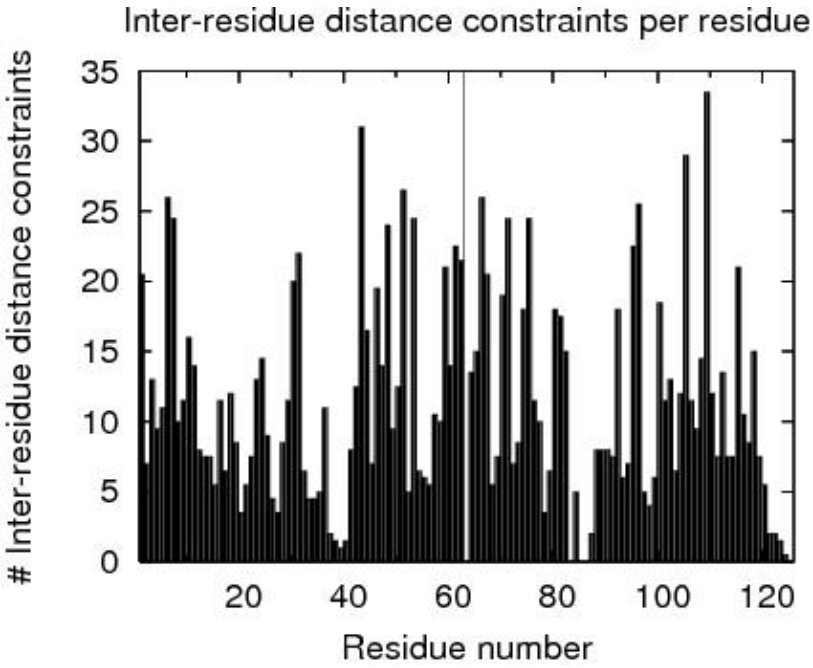
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.45	0.72	0.10	0.17	10.97
Z-score[1]	-0.16	0.29	0.71	1.01	-0.36

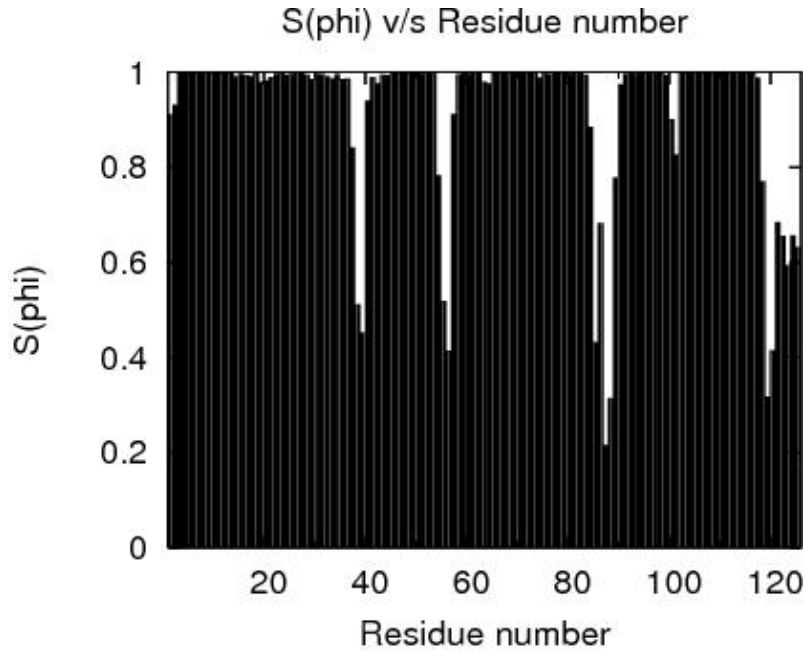
Generalized linear model RMSD prediction: 1.51

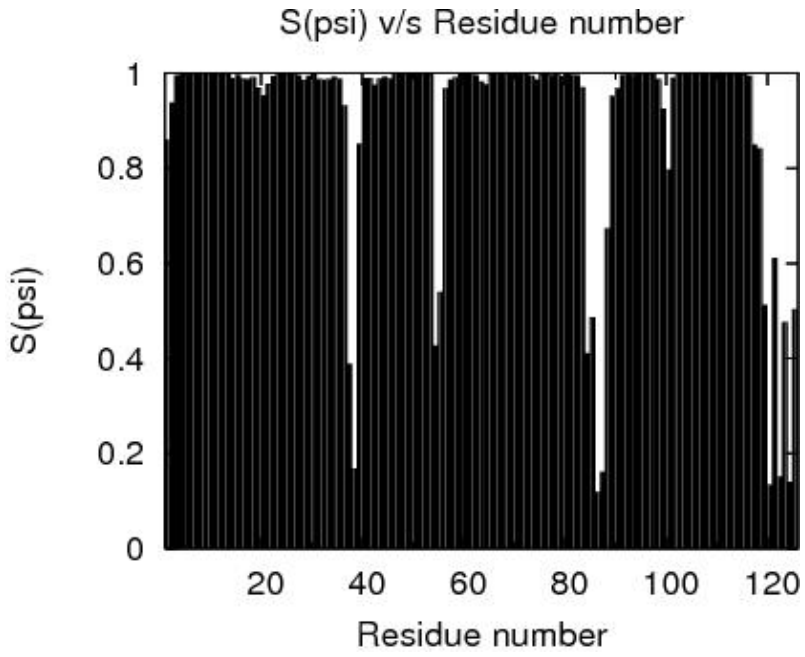
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	0
RMS deviation for bond angles:	1.2 °
RMS deviation for bond lengths:	0.018 Å

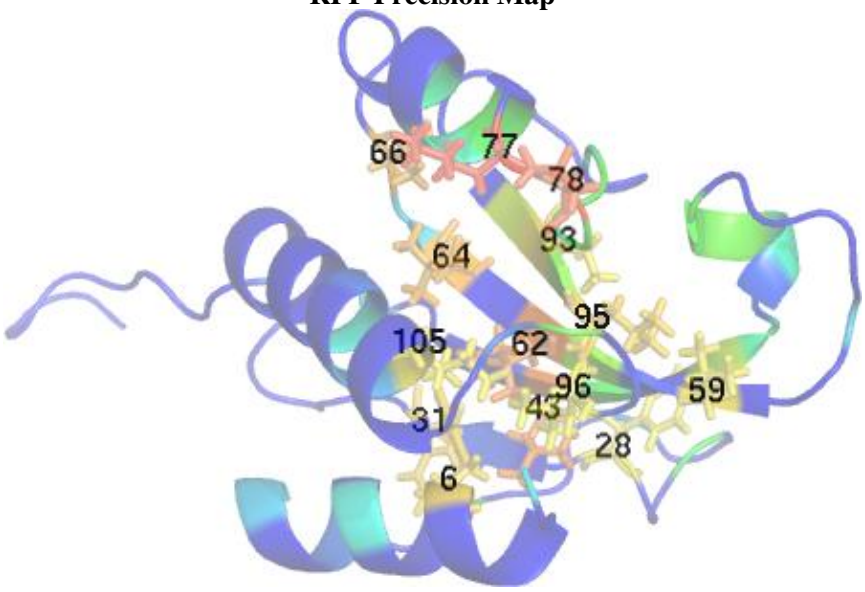
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 2A-36A,40A-53A,57A-83A,90A-99A,101A-117A
[3]Selected residues: 2A-36A,40A-53A,57A-83A,90A-99A,101A-116A


Inter-residue distance constraints per residue
Inter-residue distance constraints
0
5
10
15
20
25
30
35
20
40
60
80
100
120
Residue number

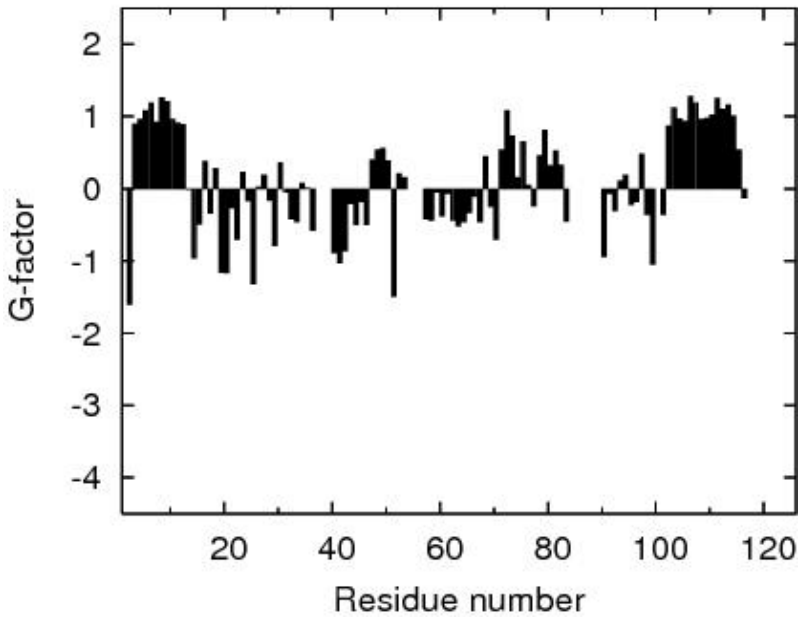

S(phi) v/s Residue number
S(phi)
0
0.2
0.4
0.6
0.8
1
20
40
60
80
100
120
Residue number



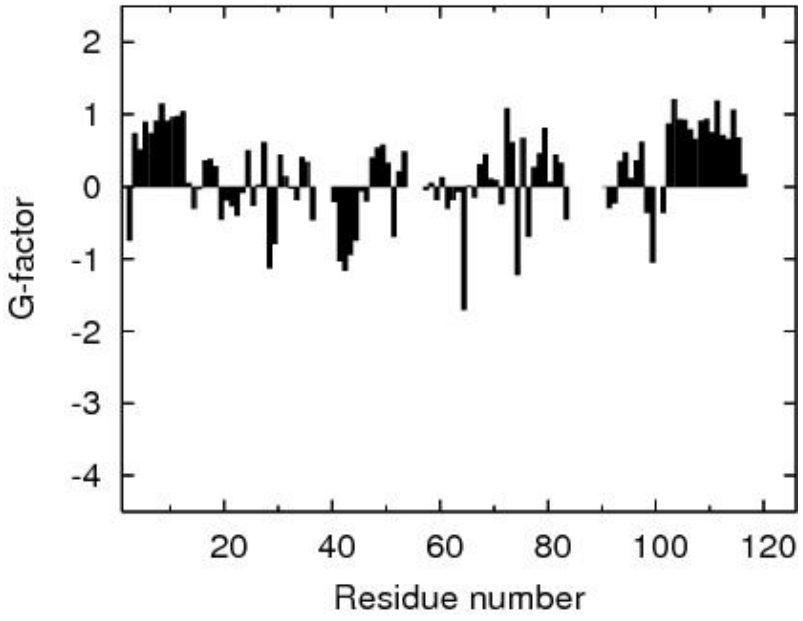
RPF Precision Map

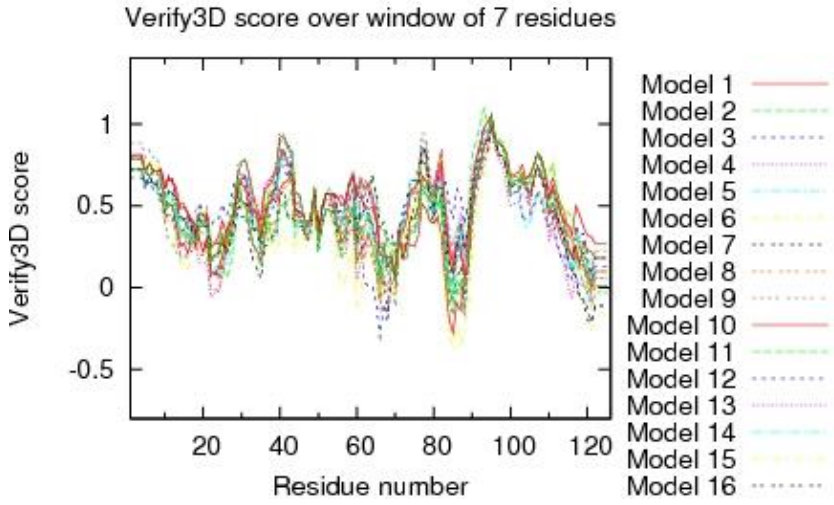


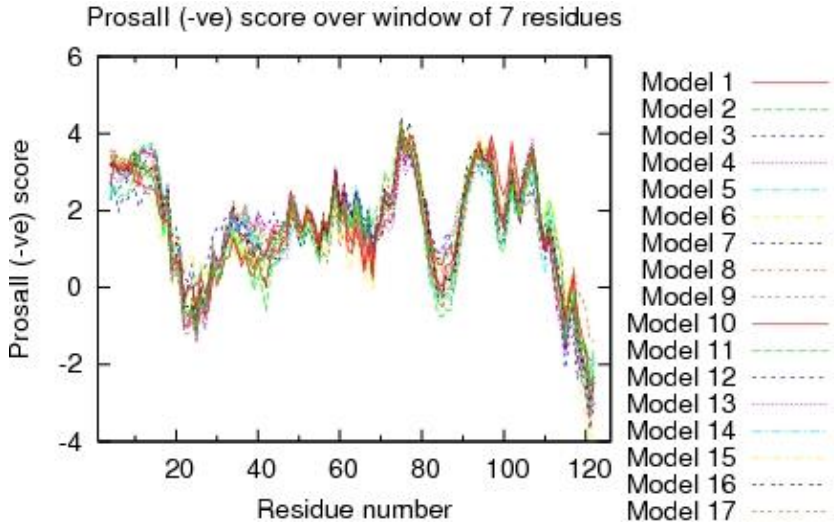
Procheck G-factor for phi-psi

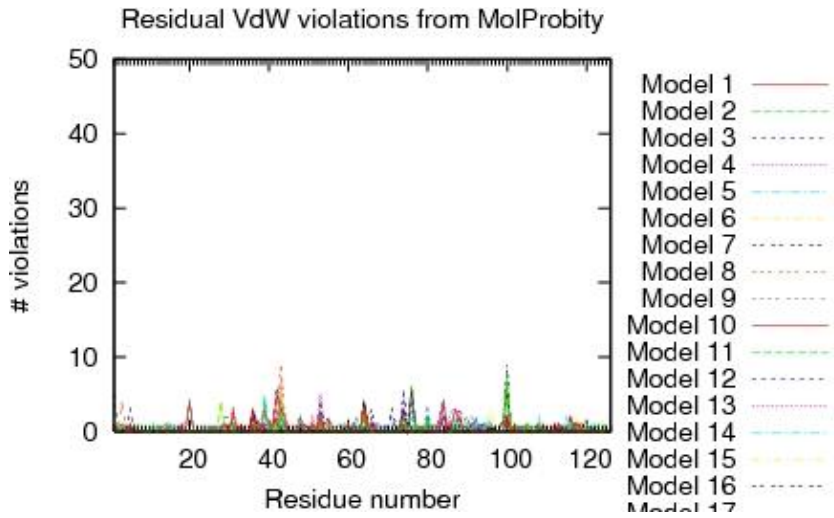


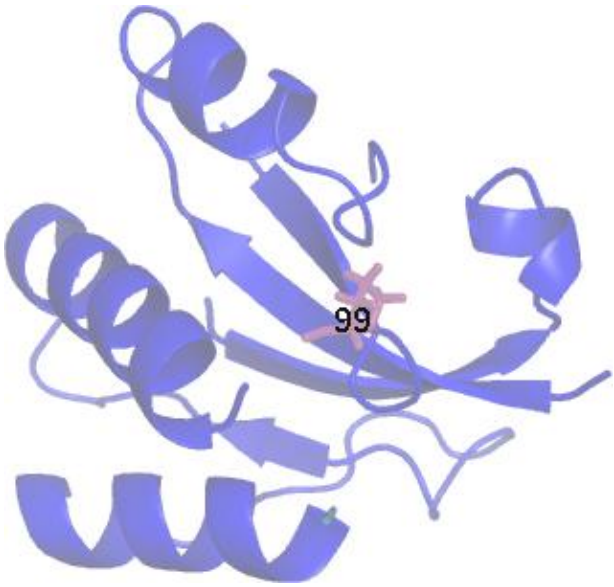
Procheck G-factor for all dihedral angles




Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
20
40
60
80
100
120
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10
Model 11
Model 12
Model 13
Model 14
Model 15
Model 16


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
20
40
60
80
100
120
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10
Model 11
Model 12
Model 13
Model 14
Model 15
Model 16
Model 17


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
20
40
60
80
100
120
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10
Model 11
Model 12
Model 13
Model 14
Model 15
Model 16



Residue Plot of Ramachandran anlysis(based on data from Richardson Lab's Molprobity)

References:

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4. Sippl M J, "Calculation of Conformation Ensembles from Potentials of Mean Force", J Mol Biol 213 (1990): 859-883
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8. Word J M et al, "Asparagine and Glutamine: Using Hydrogen Atom Contacts in the Choice of Side-chain Amide Orientation", J Mol Biol 285 (1999): 1735-1747
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Analysed by on May-10-2013 using PSVS 1.3

Software Environment

Software for structure quality evaluation:

DSSP	DsspCMBI-April-2000
pdbstat	PdbStat-5.4 Version
AutoAssign	Version 2.4.0 (uses only AVS scripts)
RPF analysis	ASDP-1.0
PDB validation	Version 8.061
Verify3D	Version 1.0 corrected by Aneerban
ProsaII	Prosa2003
PROCHECK	Version 3.5.4
MolMol	Version 2K.2

MolProbity programs:

cluster	1999
clashlistcluster	1999 (corrected by Aneerban)
mage	Version 6.35.040409
prekin	Version 6.35.040406
reduce	Version 2.14
probe	Version 2.6

Other Software:

PERL	Version 5.8.0
convert	ImageMagick 5.5.6
ps2pdf	Ghostscript 7.05
htmldoc	v1.9
gnuplot	Version 3.7 patchlevel 3

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jpegtopnm       year 2000
pnmcrop         year 2000
pnmtojpeg       year 2000
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